Real-time ray tracing of complex molecular scenes with **BALLView** and **RTfact**

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**Introduction**

Molecular viewing and editing tools are an important part of many applications and processes in structural bioinformatics, computational chemistry, and pharmacy.

A particularly important factor is to provide the user with an accurate and informative (3D) spatial representation of molecular structural arrangements. Another important goal of molecular graphics is to create publication-quality images.

To this end, ray tracing is usually the method of choice; although it traditionally takes minutes to hours to produce high-quality results.

However, recent developments in computer graphics have made real-time ray tracing of complex scenes with high visual quality become a reality.

**RTfact**

RTfact is a C++ real-time ray tracing library that utilizes generic programming concepts to deliver both performance and flexibility. The generic design allows to combine the most suitable algorithms and data structures for a specific application in order to achieve optimal performance.

RTfact handles even huge models interactively and through correct usage of shadows and lighting enhances the structural perception significantly.

**BALLView**

The Biochemical Algorithms Library (BALL) is a comprehensive and extensive rapid C++ application development framework for structural bioinformatics and molecular modelling.

It is available free of charge under the LGPL and GPL for all major operating systems. Both source code and binary packages can be found at the project web site - [http://www.ball-project.org](http://www.ball-project.org).

Albeit in a naive fashion, we can handle unstructured movement, as it occurs, e.g., in molecular dynamics simulation, interactively.

**Integration**

We present the first integration of a general purpose real-time ray tracing architecture into a molecular viewing and modelling tool by integrating the RTfact library into BALLView.

Integration of the ray tracer is done tightly and transparently, allowing advanced effects to work seamlessly with any combination of available representations in interactive speed.